ELASTIC CONSTANTS OF A STRESSED LAYER FROM SURFACE ACOUSTIC WAVE MEASUREMENTS

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INTRODUCTION

It is well known that the propagation of both bulk and surface acoustic waves (SAWs) is affected by the presence of static stresses, a phenomenon known as the acoustoelastic effect. Ultrasonic measurements of velocity therefore depend on the stresses within the material, as well the elastic constants and the density. Although the effect of stress on the velocity is small, many ultrasonic methods are sufficiently accurate to detect the changes involved. When inverting such measurements to obtain elastic constants, it is desirable to take the effect of stress into account. Similarly, when using ultrasonic methods to measure stress, it is necessary to have accurate values for the elastic constants. In practice, the material parameters of the 'natural', unstressed state are often either completely unknown or not known with sufficient accuracy (as is usually the case for residual stresses), or else cannot be assumed to be equal to bulk values (as in the case of layered materials). This is a major distinction between situations involving residual as opposed to applied stress, since a reference state of some description is always available in the latter case.

In this paper we show how to improve the estimation of the elastic constants of the natural state of a residually stressed layer from SAW measurements. To do this, we incorporate the stress into the forward calculation of the SAW velocity, so that fitting of the measured SAW dispersion then yields the elastic constants of the unstressed state. We then apply the procedure to GaAs wafers implanted with Si^+ ions.

BACKGROUND

The use of SAWs to determine material constants is particularly important for thin layers, where bulk wave measurements become more difficult. It is probably unrealistic to be able to ascertain the elastic constants, density and stress by inversion of measured SAW dispersion. Since the effect of stress on the velocity is usually small, this is the most difficult parameter to determine, as it is strongly affected by inaccuracies in the other constants. In the case of bulk waves, the presence of stress can sometimes be ascertained unambiguously. For example, when there is an anisotropic distribution of stress in the plane of interest, two orthogonally polarised shear horizontal waves propagating in this plane will travel at different velocities. Since this difference in velocity vanishes in an unstressed material, the phenomenon provides a direct indication of the presence of stress, and similar effects have been employed in various guises to map out stress distributions in materials [e.g. 1-3]. Although there are likely to be effects similar to shear wave birefringence for SAWs with predominantly shear horizontal polarisation, in most cases the effect of stress on velocity is not as clear cut, and the inverse problem is susceptible to errors in the elastic constants. In the case of residual stresses therefore, an accurate determination of the elastic constants of the unstressed state is essential.

THEORY

Acoustoelasticity

In acoustoelasticity, the infinitessimal displacements u_i associated with the ultrasonic wave are superimposed onto a static deformation of the solid, as shown schematically in figure 1. Since the static deformation may well be finite, non-linear elastic theory is required, and this necessitates three changes from familiar linear theory. Firstly, the linear strain tensor needs to be replaced by a finite strain tensor, such as the Lagrangian strain, η_{ij}:

$$\eta_{ij} = \frac{1}{2}\left(\frac{\partial u_i^s}{\partial X_j} + \frac{\partial u_j^s}{\partial X_i} + \frac{\partial u_k^s}{\partial X_i}\frac{\partial u_k^s}{\partial X_j} \right) \tag{1}$$

Secondly, Hooke's law is no longer adequate, and it is usual to postulate a hyperelastic constitutive relationship by expanding the internal energy density, W, as a function of the Lagrangian strain, η_{ij}:

$$\rho_0 W(\eta) = \tfrac{1}{2} c_{ijkl}\eta_{ij}\eta_{kl} + \tfrac{1}{6} c_{ijklmn}\eta_{ij}\eta_{kl}\eta_{mn} + \ldots \tag{2}$$

The nth order elastic constants are defined as the nth order derivatives of the energy density with respect to the strain, where the constants are evaluated at zero strain [4]. This relationship assumes that the deformation is elastic, and is therefore invalid in many cases of residual stress, although progress has been made in the development of acoustoelasticity for such cases [5,6].

Finally, the change in geometry between the undeformed and statically stressed states gives rise to various different expressions for the stress and the equation of equilibrium, depending on which coordinate system these are referred to.

The linearised equations of motion for the passage of the ultrasonic wave, when written in terms of the initial configuration, take the following form [7]

$$\left(\delta_{ik}\sigma_{jl} + C_{ijkl}\right)\frac{\partial u_k^2}{\partial x_j \partial x_l} = \rho^i \frac{\partial^2 u_i}{\partial t^2} \tag{3}$$

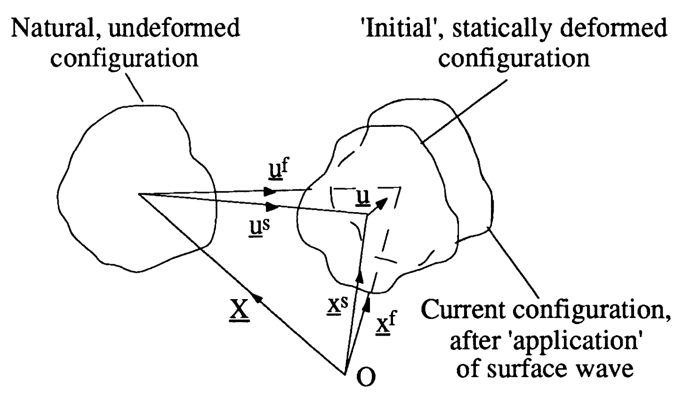

Figure 1. Relationship between natural, initial and current material configurations. The superscript on u^s is used to emphasise that this variable refers to a static, finite displacement.

where σ_{ij} is the static stress, and C_{ijkl} are modified elastic constants with the full symmetry of the second order stiffnesses . It may be noted that the stress entered into equation (3) only needs to be specified using Hooke's law for a consistent level of approximation to be maintained [8]. By retaining terms up to cubic in the strain in the expansion (2), the effective elastic constants C_{ijkl} may be written as [7] :

$$C_{ijkl} = c_{ijkl}\left(1 - e^s_{nn}\right) + c_{ijklmn}e^s_{mn} + c_{mjkl}\frac{\partial u^s_i}{\partial x_m} + c_{imkl}\frac{\partial u^s_j}{\partial x_m} + c_{ijml}\frac{\partial u^s_k}{\partial x_m} + c_{ijkm}\frac{\partial u^s_l}{\partial x_m} \tag{4}$$

where

$$e^s_{mn} = \frac{1}{2}\left(\frac{\partial u^s_m}{\partial x_n} + \frac{\partial u^s_n}{\partial x_m}\right)$$

In the case of a material that is cubic in the unstressed state and subject only to a perpendicular strain, e^s_3, as is the case for the ion-implanted material studied here, the effective elastic constants C_{IJ} may be expressed neatly in terms of the strains as

$$\begin{aligned}
C_{11} &= c_{11}\left(1 - e^s_3\right) + c_{112}e^s_3 & C_{33} &= c_{11}\left(1 + 3e^s_3\right) + c_{111}e^s_3 \\
C_{12} &= c_{12}\left(1 - e^s_3\right) + c_{123}e^s_3 & C_{44} &= c_{44}\left(1 + e^s_3\right) + c_{155}e^s_3 \\
C_{13} &= c_{12}\left(1 + e^s_3\right) + c_{112}e^s_3 & C_{55} &= c_{44}\left(1 + e^s_3\right) + c_{155}e^s_3 \\
C_{22} &= c_{11}\left(1 - e^s_3\right) + c_{112}e^s_3 & C_{66} &= c_{44}\left(1 - e^s_3\right) + c_{144}e^s_3 \\
C_{23} &= c_{12}\left(1 + e^s_3\right) + c_{112}e^s_3 & &
\end{aligned} \tag{5}$$

where reduced notation has been used.

Finally, the density of the material is altered by the deformation. To a consistent level of approximation, the density in equation (3) may be expressed in terms of that in the undeformed state as:

$$\rho^i = \rho^0\left(1 - e^s_3\right) \tag{6}$$

Implementation for SAWs

A computer program has been written to allow the calculation of SAW velocity and attenuation at the boundary between a fluid and an anisotropic, statically stressed, coated halfspace. The program allows the calculation of "pseudo" SAW type solutions that decay into the substrate, and also "leaky" SAW solutions, that decay into the fluid. These modes are particularly important in the acoustic microscope [9]. A number of techniques are available in the program to allow automatic tracking of a single dispersive SAW mode; this is particularly important when fitting calculated curves to experiment. The basic procedure follows that developed by Farnell & Adler [10] for an unstressed layer, and is described elsewhere [8]. Nalamwar & Epstein [11] have calculated velocities for a homogeneously stressed piezoelectric anisotropic layer, but their analysis is incorrect, since they did not maintain a consistent level of approximation for their effective elastic constants. Mase & Johnson [12] have presented a calculation for SAWs in a homogeneously stressed anisotropic half-space, but do not deal with attenuating modes or layers.

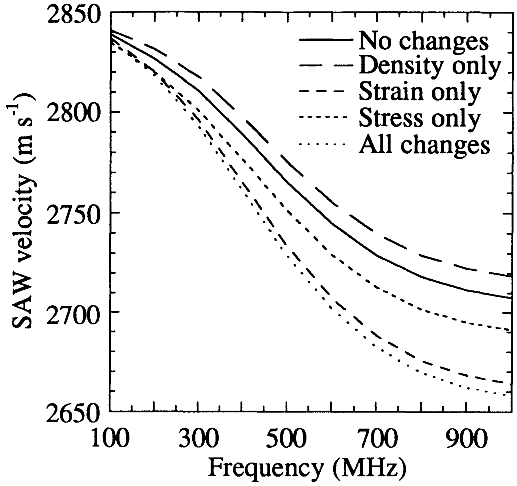

Figure 2. Calculated SAW dispersion for a strained GaAs layer on a GaAs(001) substrate, along the ⟨110⟩ direction.

Example - A Stressed Cubic Layer on a Cubic Substrate

When modelling a statically stressed material using equation (3), three separate effects must be considered. Firstly, the strain results in a change in density, as in equation (6). Secondly, the strain modifies the second order elastic constants according to equation (5). Lastly, the stress is incorporated directly into the equation of motion (3). Depending on the particular geometry, these three effects can either enhance or cancel each others contributions to the overall change in SAW velocity [11]. As a specific example, the case of a cubic layer subject to a planar stress and perpendicular strain, bonded to an unstressed infinite substrate is now considered.

Figure 2 shows SAW dispersion curves calculated along a ⟨110⟩ type direction for a modified GaAs(001) layer on a pure GaAs(001) substrate. The layer is subject to a perpendicular strain of 0.4% and a planar stress of 470 MPa. Its thickness is 1.5 μm and c_{11}, c_{12} and c_{44} have been decreased by 4%, 0% and 12% respectively from the bulk values for GaAs. The figure shows that the largest single effect is due to the modification of the stiffness by the strain. The stress also tends to decrease the velocity, although to a lesser extent. The density decrease, on the other hand, causes an increase in SAW velocity when taken in isolation. The separate contributions to the net SAW velocity have implications for a potential inversion procedure, in that neglecting one or more of them will result in a 'biased' fitted set of elastic constants. By the same token, if the stress and strain can be measured and/or calculated independently, then the true elastic constants of the reference state of the layer material can be inverted. This is the approach taken in this paper for ion-implanted GaAs.

EXPERIMENTAL

GaAs wafers were implanted at room temperature with Si^+ ions at energies of 0.5, 1.5 and 4 MeV. The dose was fixed at a value of 10^{14} ions cm^{-2}, such that the implanted region was still crystalline. This was confirmed by X-ray triple crystal diffractometry, which was used to determine the strain [13].

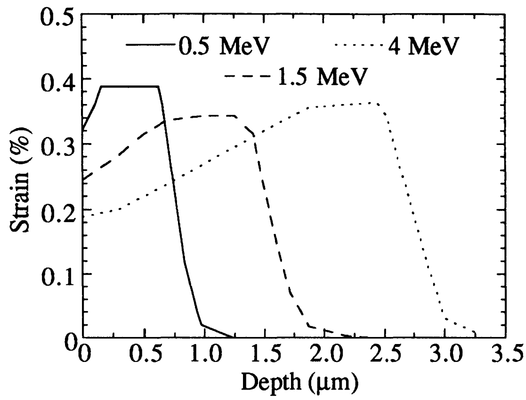

Figure 3. Perpendicular strain depth profile measured by DC diffractometry in ion implanted GaAs(001) samples.

The implanted region was modelled as a single cubic layer subject to a compressive planar stress and a perpendicular expansive strain, on a substrate of unmodified GaAs. The measured strain profiles are shown in figure 3, and demonstrate that the use of a single layer is a good approximation except at the highest energy, where the damaged layer is buried below the surface.

Measurements of SAW velocity were made using the line-focus beam (LFB) acoustic microscope [14]. The use of a cylindrical acoustic lens enables directional excitation of SAWs, and hence measurements on anisotropic materials. Other advantages of the acoustic microscope over other methods of SAW excitation are the high measurement accuracy (~0.1–0.5%) and the ease of use. The SAW velocity is inferred from oscillations in the microscope output that occur as the specimen is brought towards the lens from focus, a curve known as the $V(z)$. A discussion of the analysis of the $V(z)$ to obtain SAW velocities may be found elsewhere [8]. Measurements were made as a function of azimuthal angle, at a fixed frequency of 225 MHz, and are shown in figure 4.

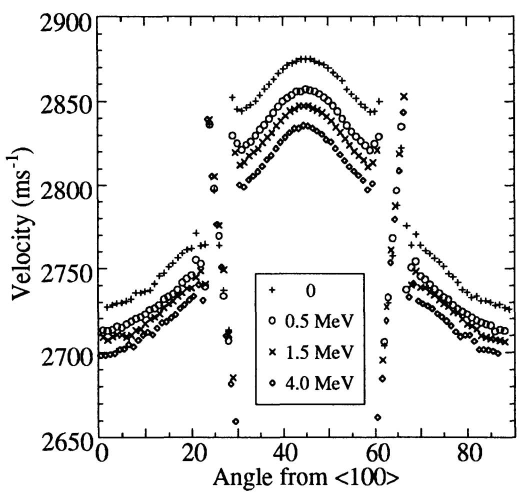

Figure 4. SAW velocity as a function of propagation direction as measured with LFB acoustic microscopy for ion implanted GaAs(001) wafers.

RESULTS AND DISCUSSION

Fitting Procedure

Fitting theory to experimental SAW data presents a number of practical problems, and most of these stem from the absence of an analytic expression for the velocity of a surface wave. The program developed here applies a non-linear least squares fit of theory to measurements of SAW angular or frequency dispersion made by any technique. The method is difficult to implement and is computationally expensive, but has the advantage of allowing a quantitative assessment of the errors in the fitted elastic constants [8]. A number of other methods, some of which are specific to acoustic microscopy, have been used to reduce the computational burden [15-17], and their merits are discussed elsewhere [8,17].

The fitting procedure begins with an initial guess at the three elastic constants for the cubic implanted material. The measured perpendicular strain is then used to calculate modified constants using equation (5). The actual tetragonal nature expected of the strained material arises naturally in these modified constants. The requirement for the third order elastic constants in equation (5) presents difficulties, in that these may well be completely unknown in general. In the present study, the implantation produces a damaged, but still crystalline layer, and we keep the third order constants fixed at the literature values for unimplanted GaAs [18]. The compressive planar stress is then calculated by analogy with a thermoelastic problem, giving [13]

$$\sigma_1 = \sigma_2 = -\varepsilon_3 \frac{c_{11}^2 + c_{11}c_{12} - 2c_{12}^2}{c_{11} + c_{12}}. \tag{7}$$

The stress is entered directly into the equation of motion (3), together with the new density, which is obtained using equation (6). SAW velocities are then calculated as a function of angle in the (001) plane, and the sum of squares of residuals evaluated. A non-linear least squares routine then attempts to minimise this sum by improving the guesses at the elastic constants.

Once a best fit has been found, the quality of this fit is checked by evaluating the RMS deviation, and by looking for trends in the residuals [19]. The covariance matrix can be estimated using the best fit parameters. The diagonal values of this matrix have been used in this work to indicate the variance in the fitted parameters, although strictly speaking this requires the error distribuation to be normal [20]. Even when the error distribution is not known to be normal, large values of the diagonal elements indicate a shallow minimum in the sum of squares of residuals, and hence insensitivity of the fit to one or more parameters. It was found that the variance in c_{12} was an order of magnitude or more higher than for c_{11} or c_{44}, which indicates that the SAW velocity in the (001) plane is relatively insensitive to c_{12}. The fitting routine can therefore easily distort this constant without altering the residual sum by a great deal. We therefore present the anisotropy ratio, $A = 2c_{44}/(c_{11}-c_{12})$, since this is subject to a smaller degree of error.

Fitting was restricted to points within 10-15° of the symmetry directions, since the analysis becomes more error prone when the SAW and pseudo SAW branches are both significantly excited. A fixed offset of 4.9 m s^{-1} was used to take account of fluid loading, this value being almost constant over the range of angles considered. With fitting restricted to 10-15° degrees of $\langle 110 \rangle$, the velocity of the true pseudo SAW lies very close to that obtained without incorporating attenuation into the calculation. These two simplifications help to keep down the computation time by avoiding the use of 2-D minimisation as required for the exact calculation of attenuating SAWs.

Since the implanted region has similar elastic constants to the substrate and is thin compared to the SAW wavelength (1.5 μm compared to 12 μm), the layer causes a relatively small perturbation to the SAW velocity of the substrate. The inversion of the elastic constants of the layer is therefore very sensitive to the values used for the substrate. It is also known

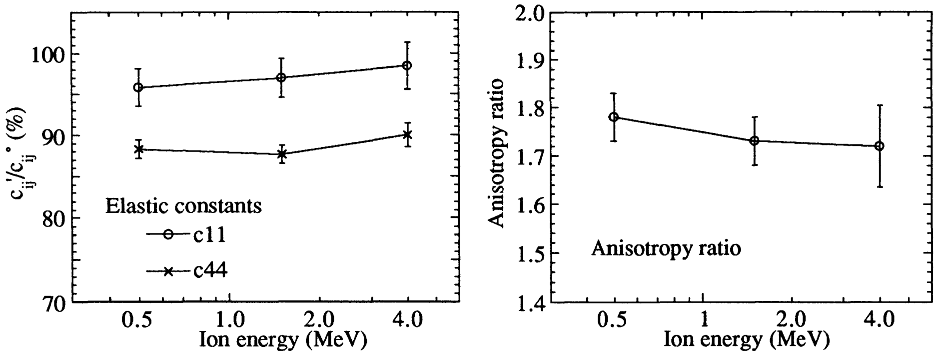

Figure 5. Estimated elastic constants and anisotropy ratio of the damaged region for GaAs implanted at room temperature with Si^+ ions. The anisotropy ratio of the unimplanted GaAs is 1.86.

that the analysis procedure can introduce distortion into the shape of angular scans [8]. Hence, rather than use literature values for the substrate second order elastic constants, we fitted elastic constants to the rotational scan for unimplanted GaAs, and used these values in all subsequent fitting for the implanted specimens.

A summary of the results is shown in figure 5. The values obtained for c_{11} and c_{44} are constants to within the errors associated with fitting, representing an average decrease of 3.5% and 12.5% respectively. The difference in the measured velocities seen in figure 4 is thus almost entirely a thickness effect, i.e. implantation at a fixed dose is creating a layer with elastic constants approximately independent of energy. The sample implanted at 4 MeV does not quite fit this trend, in that if the elastic constants fitted for the other materials are used to calculate expected velocities for the 4 MeV sample, these are about 15 m s^{-1} lower than those actually measured. The measured velocity would occur for a thickness of 2.1 μm, rather than the value of 2.7 μm actually used. This is consistent with the buried nature of the layer at 4 MeV, as seen in the strain profile in figure 3. Use of the full value of 2.7 μm for fitting is an overestimate, which has therefore resulted in an underestimate of the decrease in the elastic constants.

CONCLUSION

Accurate knowledge of the elastic constants of a material is essential if SAW measurements are to be used to estimate residual stresses. We have shown that the 'natural' elastic constants of a residually stressed anisotropic layer can be estimated by incorporating the stress directly into the equations of motion when fitting measurements of SAW dispersion. The use of a direct fit of SAW theory to experiment enables a quantitative assessment of the uncertainty in the elastic constants.

As an example, the method was applied to SAW measurements made with the line-focus beam acoustic microscope on GaAs wafers implanted with Si^+ ions. We found that for a dose of 10^{14} ions cm^{-2}, the stiffnesses c_{11} and c_{44} of the 'natural' state of the implanted material decreased on average by 3.5% and 12.5% respectively, independent of the ion energy.

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